Curriculum Vitae

PROF. GAUTAM R. DESIRAJU

School of Chemistry, University of Hyderabad, Hyderabad 500 046

E-mail: gautam_desiraju@yahoo.com Phone: 91 40 23134828

Fax: 91 40 23010567

Web Page: http://202.41.85.161/~grd/

Born

21 August 1952, in Madras

Education

B.Sc.	St. Xavier's College, University of Bombay	1972
M.S.	University of Illinois, Urbana	1974
Ph.D.	University of Illinois, Urbana	1976

Research interests Organic chemistry, Crystal engineering

Supramolecular chemistry, Drug design Pharmaceutical development, formulation Molecular modelling, crystallography

Positions held

Research Scientist	Eastman Kodak, Rochester	1976-1978
Research Fellow	Indian Institute of Science, Bangalore	1978-1979
Lecturer	University of Hyderabad	1979-1984
Reader	University of Hyderabad	1984-1990
Visiting Scientist	Dupont CR&D, Wilmington	1988-1989
Professor	University of Hyderabad	1990-
Dean	University of Hyderabad	1999-2002

Publications

2 books, 3 edited books and more than 275 research papers

- (1) Crystal Engineering. The Design of Organic Solids, Elsevier, 1989.
- (2) The Weak Hydrogen Bond, Oxford University Press, 1999 (with T. Steiner).

Honours and distinctions

- 1. Fellow, Indian Academy of Sciences, 1993.
- 2. Fellow, Indian National Science Academy, 2000.
- 3. Fellow, The National Academy of Sciences, India, 2000.
- 4. Fellow, Third World Academy of Sciences, 2002.
- 5. Fellow, Andhra Pradesh Akademi of Sciences, 1995.
- 6. Alexander von Humboldt Research Award, 2000.
- 7. Third World Academy of Sciences (TWAS) Award, 2000.
- 8. Ranbaxy Award for Pharmaceutical Sciences, 2000.
- 9. Millenium Medal of the Indian Science Congress, 2000.
- 10. Silver Medal for excellence of the Chemical Research Society of India, 2000.
- 11. CHEMITO Award, 1999.
- 12. Prof. Priyadaranjan Ray Memorial Award (Indian Chemical Society), 2000.
- 13. Dr. K. Anji Reddy Innovator of the Year Award (Indian Institute of Chemical Engineers), 2002.
- 14. Erskine Professor, University of Canterbury, Christchurch, New Zealand, 1990.
- 15. Visiting Professor, University of Strasbourg, Strasbourg, France, 1997.
- 16. Michael Visiting Professor, Weizmann Institute of Science, Israel, 2002.
- 17. Senior Visiting Fellow, Institute of Advanced Study, University of Bologna, Italy, 2003
- 18. J. C. Bose Fellowship, Department of Science and Technology, 2006.
- 19. Honorary Member, Hungarian Chemical Society, 2006.

Selected committee memberships

- 1. Executive Committee, International Union of Crystallography.
- 2. Bookseries Committee, International Union of Crystallography.
- 3. Council, Indian National Science Academy.
- 4. Research Council, Regional Research Laboratory, Thiruvananthapuram.
- 5. Management Board, National Centre for Biological Research, Bangalore.
- 6. Research Council, National Institute for Pharmaceutical Education and Research, Chandigarh.
- 7. Board of Governors, Indian Institute of Science Education and Research, Kolkata.

Selected former committee memberships

- 1. Research Council, National Chemical Laboratory, Pune.
- 2. Research Council, Indian Institute of Chemical Biology, Kolkata.
- 3. Chairman, Program Advisory Committee for Organic Chemistry, Department of Science and Technology, New Delhi.
- 4. Appellate Authority, Andhra Pradesh Pollution Control Board, Hyderabad.
- 5. National Millenium Initiative for Technology Leadership Initiatives, High Power Committee, Council of Scientific and Industrial Reseach, New Delhi.

Current and former editorial boards and editorial advisory boards

- 1. Accounts of Chemical Research (American Chemical Society).
- 2. Chemistry. An Asian Journal (Wiley-VCH).
- 3. Acta Crystallographica (International Union of Crystallography)
- 4. Crystal Growth and Design (American Chemical Society)
- 5. CrystEngComm (Royal Society of Chemistry).
- 6. Journal of Chemical Sciences (Indian Academy of Sciences).
- 7. Journal of Chemical Crystallography (Kluwer).
- 8. Encyclopedia of Supramolecular Chemistry (Marcel Dekker)
- 9. Current Opinion in Solid State and Materials Science (subject editor)
- 10. Perspectives in Supramolecular Chemistry (Wiley).
- 11. Chemical Communications (Royal Society of Chemistry)
- 12. Topics in Stereochemistry (Wiley).

Selected plenary and keynote lectures

- 1. 10th International Conference of the Chemistry of the Organic Solid State, Vancouver, Canada, 1991.
- 2. British Crystallographic Association Spring Meeting (keynote) Manchester, England, 1993.
- 3. Computational Methods in Chemical Design. Theory and Experiment (CMCD 4) Kloster Irsee, Germany, 1994.
- 4. Symposium on Organic Crystal Chemistry, Adam Mickiewicz University Poznan-Rydzyna, Poland, 1994.
- 5. NATO-ARW workshop on Crystals as Supramolecular Materials, Sestre Levante, Italy, 1995.
- 6. 2nd Meeting of the Asian Crystallographic Association (keynote) Bangkok, Thailand, 1995.
- 7. NATO-ARW workshop on Self Assembly in Synthetic Chemistry, Val Morin, Québec, Canada, 1996.
- 8. Summer School on Supramolecular Chemistry Ustrón, Poland, 1996.
- 9. International Union of Crystallography XVII Congress (keynote) Seattle, U.S.A., 1996.
- 10. XIIIth International Symposium on the Reactivity of Solids (keynote) Hamburg, Germany, 1996.
- 11. NATO-ASI school on Crystal Engineering, Digby, Nova Scotia, Canada, 1996.
- 12. Analysis and Design of Solid State Reactions, Tokyo Institute of Technology Tokyo, Japan, 1996.
- 13. 36th IUPAC Congress (keynote) Geneva, Switzerland, 1997.
- 14. NATO-ARW on Large Supramolecular Assemblies Athens, Greece, 1997.

- 15. NATO-ARW on Molecular Magnets and Conductors Barcelona, Spain 1998.
- 16. Royal Society of Chemistry Annual Congress (Symposium on Polymorphism) Durham, England 1998.
- International School of Crystallography and NATO-ARW
 Implications of Molecular and Materials Structure for New Technologies
 Ettore Majorana Centre for Scientific Culture
 Erice, Sicily, Italy, 1998.
- 18. American Crystallographic Association Annual Meeting (Invited speaker in the symposium to commemorate the 50th anniversary of the Internation Union of Crystallography) Arlington, VA, U.S.A., 1998.
- Design and Assembly of Molecules and Networks: New Forms and Functions Cursos de Verano Universidad Complutense San Lorenzo de el Escorial, Spain, 1998.
- 20. Gordon Conference on Physical Organic Chemistry Fukuoka, Japan, 1998.
- 21. 16th International CODATA Conference New Delhi, India, 1998.
- Sonderforschungsbericht programme in Supramolecular Chemistry (Universities of Essen and Bochum) Essen, Germany, 1998.
- 23. International School of Crystallography and Euroconference Crystal Engineering: From Molecules and Crystals to Materials Ettore Majorana Centre for Scientific Culture Erice, Sicily, Italy, 1999.
- International School of Crystallography
 Data Mining in Crystallography
 Ettore Majorana Centre for Scientific Culture
 Erice, Sicily, Italy, 1999.
- 25. Drug Design and Small-molecule Crystallography Technical University of Łodz, Łodz, Poland, 1999.
- 26. Royal Society of Chemistry Symposium on Crystal Engineering and Supramolecular Chemistry (keynote) London, England, 1999.
- 27. Foundation Day Lecture
 National Institute of Immunology
 New Delhi, 2001.
- 28. Indian Association for the Cultivation of Science, 125th anniversary lecture IACS, Kolkata, 2001.
- 29. Department of Atomic Energy-C.V. Raman Lectureship Institute of Science and St. Xavier's College, Mumbai, 2001.
- 30. American Chemical Society Annual Meeting (keynote)

- Orlando, Florida, 2002
- 31. American Crystallographic Association Annual Meeting (keynote) San Antonio, Texas, 2002.
- 32. Third World Academy of Sciences Annual Meeting (award lecture) New Delhi, 2002.
- 33. Prof. Priyadaranjan Ray Memorial Award Lecture (Indian Chemical Society) Nagarjuna University, Guntur, 2002.
- 34. Foundation Day Lecture Institute of Microbial Technology Chandigarh, 2003.
- 35. American Chemical Society ProSpectives Series on Polymorphism Tampa, Florida, 2003.
- 36. Foundation Day Lecture Central Salt and Marine Chemicals Research Institute Bhavnagar, 2003.
- 37. European Crystallographic Meeting Durban, 2003.
- 38. American Chemical Society ProSpectives Series on Polymorphism Tampa, Florida, 2004.
- 39. Scientific Update conference on polymorphism New Orleans, 2004.
- 40. American Crystallographic Association Orlando, Florida, 2005
- 41. Singapore International Chemists Conference (SICC-4) Singapore, 2005 (plenary).

Summary

Gautam R. Desiraju (b. 1952 in Madras) studied chemistry at the Universities of Bombay and Illinois. He has been at the University of Hyderabad since 1979 and has made seminal contributions to the growth and development of the subject of crystal engineering, with particular reference to the properties of the weak hydrogen bond and the use of logic based retrosynthesis with supramolecular synthons. He has written more than 275 scientific papers and is the author of the definitive work Crystal Engineering. The Design of Organic Solids (Elsevier, 1989) and The Weak Hydrogen Bond in Structural Chemistry and Biology (with T. Steiner, OUP, 1999). He has lectured widely and is a recipient of the Alexander von Humboldt Forschungspreis (2000). He has been a Michael Visiting Professor in the Weizmann Institute of Science (2002), a holder of a Short Term Visiting Fellowship of the Japan Society for the Promotion of Science (2003) and a Senior Visiting Fellow in the Institute of Advanced Study, University of Bologna (2003). He is presently a member of the Executive Committee of the International Union of Crystallography. He is a consulting editor for Accounts of Chemical Research, a coeditor of Acta Crystallographica, and is on the editorial advisory boards of a large number of journals, including most recently Chemistry-An Asian Journal.

Publication List for Guatam R. Desiraju

BOOKS

- 1. Organic Solid State Chemistry, edited by G. R. Desiraju, Studies in Organic Chemistry 32, Elsevier, Amsterdam, 1987: multi-author work with 16 chapters, 550 pages.
- 2. Crystal Engineering. The Design of Organic Solids by G. R. Desiraju, Materials Science Monographs 54, Elsevier, Amsterdam, 1989: 312 pages.
- The Crystal as a Supramolecular Entity edited by G. R. Desiraju, Perspectives in Supramolecular Chemistry, 2, Wiley, Chichester, 1996: multi-author work with 6 chapters, 309 pages.
- 4. The Weak Hydrogen Bond in Structural Chemistry and Biology by G. R. Desiraju and T. Steiner, Oxford University Press, Oxford, 1999: 528 pages.
- Crystal Design. Structure and Function edited by G. R. Desiraju, Perspectives in Supramolecular Chemistry, 7, Wiley, Chichester, 2003: multi-author work with 9 chapters, 408 pages.

Scientific Literature Publications

- Conversion in the solid state of the yellow to the red form of 2-(4-methoxyphenyl)-1,4benzoquinone. X-ray crystal structures of the two forms and anisotropy of the rearrangement.
 - G. R. Desiraju, I. C. Paul and D. Y. Curtin
 - J. Am. Chem. Soc., 99, 1594-1601 (1977).
- 2. Crystal growth by non-aqueous gel diffusion.
 - G. R. Desiraju, D. Y. Curtin and I. C. Paul
 - J. Am. Chem. Soc., 99, 6148 (1977).
- 3. Synthesis and interconversion by hydrogen exchange of isomeric quinhydrones.
 - G. R. Desiraju, D. Y.Curtin and I. C. Paul
 - J. Org. Chem., 46, 4071-4075 (1977).
- 4. Resonance interactions in metal chelates of ortho-hydroxyazo compounds. Crystal growth, Structure and Spectra of 1-(2-Pyridylazo)-2-naphtholato-copper (II).
 - G. R. Desiraju, H. R. Luss and D. L. Smith
 - J. Am. Chem. Soc., 100, 6375-6382 (1978).
- 5. Structure studies of 1:1 quinone-hydroquinone complexes.
 - G. R. Desiraju, I. C. Paul and D. Y. Curtin
 - Mol. Cryst. Liq. Cryst., 52, 259-266 (1979).
- Phase transition in malonic acid; an infrared study.
 S. Ganguly, J. R. Fernandes, G. R. Desiraju and C. N. R. Rao Chem. Phys. Lett., 69, 227-229 (1980).

7. Organic solid state chemistry-I. Topochemistry.

G. R. Desiraju

Indian J. Chem. Ed., 7(1), 1-8 (1980).

8. Organic solid state chemistry-II. Non-topochemical processes.

G. R. Desiraju

Indian J. Chem. Ed., 7(2), 1-6 (1980).

 Phase transitions in solid hydrogen bonded p-chlorobenzamide, p-nitrophenol and an azo dye.

S. Ganguly and G. R. Desiraju

Indian J. Chem., 20A, 80-81 (1981).

 Organic reactions in inorganic matrices-oxidation of hydroquinone to p-benzoquinone on solid MoO3 surfaces.

G. R. Desiraju and B. P. Shastry

Proc. Indian Acad. Sci. (Chem. Sci.), 90, 243-246 (1981).

11. A mild transformation of g -FeOOH to g -Fe2O3 using organic reagents.

G. R. Desiraju and M. Rao

Mat. Res. Bull., 17, 443-449 (1982).

12. 6-Chloro-4-phenyl-1-methyl-2,1,3-benzothiadiazine-2,2-dioxide.

G. R. Desiraju and R. Kamala

Acta Crystallogr., Section C, 39, 358-360 (1983).

13. Intermolecular proton transfers in the solid state: conversion of the hydroxyazo to the quinonehydrazone tautomer of 2-amino-3-hydroxy-6-phenylazopyridine. X-ray crystal structures of the two forms.

G. R. Desiraju

J. Chem. Soc., Perkin Transac. 2, 1025-1030 (1983).

14. Crystal engineering via donor-acceptor interactions. X-ray crystal structure and solid state reactivity of the 1:1 complex 3,4-dimethoxycinnamic acid-2,4-dinitrocinnamic acid.

J. A. R. P. Sarma and G. R. Desiraju

J. Chem. Soc., Chem. Commun., 45-46 (1983).

15. Structural mimicry and the photoreactivity of organic solids.

W. Jones, C. R. Theocharis, J. M. Thomas and G. R. Desiraju

J. Chem. Soc., Chem. Commun., 1443-1444 (1983).

 Crystal engineering via non-bonded interactions involving oxygen. X-ray crystal structures of 3,4-methylenedioxycinnamic acid and 3,4-dimethoxycinnamic acid.

G. R. Desiraju, R. Kamala, B. H. Kumari and J. A. R. P. Sarma

J. Chem. Soc., Perkin Transac. 2, 181-189 (1984).

17. Crystal engineering via CI????CI non-bonded interactions. The novel 2:1 complex 6-chloro-3,4-methylenedioxycinnamic acid - 2,4-dichlorocinnamic acid. Topochemical conversion to an unsymmetrical cyclobutane and kinetics of the reaction.

J. A. R. P. Sarma and G. R. Desiraju

J. Chem. Soc., Chem. Commun., 145-147 (1984).

18. Organic solid state chemistry - some perspectives.

G. R. Desiraju

Proc. Indian Acad. Sci. (Chem. Sci.), 93, 407-419 (1984).

 An NMR method to distinguish between truxinic and truxillic dimers of some trans-cinnamic acids.

J. A. R. P. Sarma and G. R. Desiraju Indian J.Chem., B23, 658-659 (1984).

20. The use of mixed crystals for engineering organic solid state reactions : applications to benzylbenzylidenecyclopentanones.

C. R. Theocharis, G. R. Desiraju and W. Jones

J. Am. Chem. Soc., 106, 3606-3609 (1984).

21. An investigation into the role of chloro-substituents in hydrogen bonded crystals: the crystal structures of the dichlorophenols.

N. W. Thomas and G. R. Desiraju

Chem. Phys. Lett., 110, 99-102 (1984).

22. Carrying out organic chemistry within crystalline solids

G. R. Desiraju

Endeavour, 8, 201-206 (1984).

23. Determination of an organic crystal structure with the aid of topochemical and related considerations: correlation of the molecular and crystal structures of a -benzylidene-g -butyrolactone and 2-benzylidenecyclopentanone with their solid state photoreactivity. S. K. Kearsley and G. R. Desiraju

Proc. Roy. Soc. London Ser.A, 397, 157-181 (1985).

24. The chloro-substituent as a steering froup: a comparative study of non-bonded interactions and hydrogen bonding in crystalline chloro-aromatics.

J. A. R. P. Sarma and G. R. Desiraju Chem. Phys. Lett., 117, 160-164 (1985).

25. Organische Chemie in kristallinen Festk?rn.

G. R. Desiraju

Die Umschau, 413-417 (1985).

26. The novel 1:1 donor acceptor complex 3,4-dimethoxycinnamic acid - 2,4-dinitrocinnamic acid. Crystal engineering, structure and anomalous lack of solid state topochemical reactivity.

J. A. R. P. Sarma and G. R. Desiraju

J. Chem. Soc., Perkin Transac. 2, 1905-1912 (1985).

27. Some chemical implications of database derived crystallographic information.

G. R. Desiraju

Indian J.Chem., B25, 1-8 (1986).

What is the maximum yield in the solid state cinnamic acid dimerisation? A combinatorial mathematical approach.

G. R. Desiraju and V. Kannan

Proc. Indian Acad. Sci. (Chem. Sci.), 96, 351-362 (1986).

29. Crystal engineering and chemical reactivity of organic molecular solids.

G. R. Desiraju

Proc. Indian Natnl. Sci. Acad., 52A, 379-399 (1986).

30. The chloro-methyl exchange rule and its violations in the packing of organic molecular solids.

G. R. Desiraju and J. A. R. P. Sarma

Proc. Indian Acad. Sci. (Chem. Sci.), 96, 599-605 (1986).

31. Molecular discrimination in the formation of mixed crystals of some substituted chlorocinnamic acids.

J. A. R. P. Sarma and G. R. Desiraiu

J. Am. Chem. Soc., 108, 2791-2793 (1986).

32. Recent studies on the formation and properties of quinhydrone complexes. A. O. Patil, W. T. Pennington, G. R. Desiraju, D. Y. Curtin and I. C. Paul, Mol. Cryst. Liq. Cryst., 134, 279-304 (1986).

33. The role of non-bonded interactions involving sulphur in the crystal engineering of 4ŭshort axis structures. Unusual topochemical reactivity of 4-(4-chlorophenyl)thiazole-2(1H)-thione. V. Nalini and G. R. Desiraju

J. Chem. Soc., Chem. Commun., 1030-1032 (1986).

34. The role of CI????CI and C- H????O interactions in the crystal engineering of 4Š- short axis structures.

J. A. R. P. Sarma and G. R. Desiraju

Acc. Chem. Res., 19, 222-228 (1986).

35. Hydrogen bonding and phase transitions in pentachlorophenol - hexachlorobenzene solid solutions.

Md. A. Masood and G. R. Desiraju

Chem. Phys. Lett., 130,199-202 (1986).

36. Dipole-dipole interactions and the inversion motif in the crystal structures of planar chloro aromatics: the unusual packings of 1,2,3-trichlorobenzene and 1,2,3,7,8,9hexachlorodibenzo-p-dioxin.

G. R. Desiraju, J. A. R. P. Sarma and T. S. R. Krishna

Chem. Phys. Lett., 131,124-128 (1986).

37. Interstack and intrastack forces in molecular solids: a new look at donor-acceptor complexes and organic metals.

G. R. Desiraju

Curr. Sci. (India), 55, 1009-1012 (1986).

38. Structure of 3-hydroxy-6-(4-methyl)phenylazopyridine.

T. S. R. Krishna and G. R. Desiraju

Acta Crystallogr., Section C, 42, 1246-1248 (1986).

39. Crystal engineering, X-ray crystallography and organic solid state chemistry G. R. Desiraju

Indian J.Phys., 61A, 43-50 (1987).

40. The crystal and molecular structure of 3,4-dihydroxy-trans-cinnamic acid, C₉H₈O₄, caffeic acid and its lack of solid state topochemical reactivity.

S. Garcia-Granda, G. Beurskens, P. T. Beurskens, T. S. R. Krishna and G. R. Desiraju

Acta Crystallogr., Section C, 43, 683-685 (1987).

41. Crystal engineering through non-bonded contacts to sulphur. Structure and solid state photoreactivity of 4-(4'-chloro)phenyl-D -4-thiazolene-2-thione.

V. Nalini and G. R. Desiraju

Tetrahedron, 43, 1313-1320 (1987).

- 42. Gas-solid reaction of 4-phenylthiazole-2(1H)-thione.
 - V. Nalini and G. R. Desiraiu
 - J. Chem. Soc., Chem. Commun., 1046-1048 (1987).
- 43. Crystal engineering a 4 ŭshort axis for planar chloro aromatics:
 - G. R. Desiraju in Organic Solid State Chemistry, Ed. G. R. Desiraju, Elsevier, Amsterdam (1987), pp 519-546.
- Correlation between crystallographic and spectroscopic properties for C- H????O bonds in terminal acetylenes.
 - G. R. Desiraju and B. N. Murty

Chem. Phys. Lett., 139, 360-361 (1987).

- 45. Mixed crystals of 6-chloro-3,4-methylenedioxycinnamic acid with 2,4- and 3,4- dichlorocinnamic acids. Structure, topochemistry and intermolecular interactions.
 - J. A. R. P. Sarma and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 1187-1193 (1987).
- 46. C- H????O interactions and the adoption of 4ŭshort axis structures by oxygenated aromatic compounds.
 - J. A. R. P. Sarma and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 1195-1202 (1987).
- 47. Designing organic crystals.
 - G. R. Desiraju

Prog. Solid State Chem., 17, 295-353 (1987).

- 48. Crystal engineering a solid state Diels-Alder reaction.
 - K. V. R.Kishan and G. R. Desiraju
 - J. Org. Chem., 52, 4640-4641 (1987)
- Structure and photochemical reactivity of some chlorocinnamic acid molecular complexes.
 R. Desiraiu

Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk, 15-21 (1987).

- Structure of (4 SR, 6a RS)-4-[-2-methyl-1,3-dioxalan-2-yl)ethyl]-4,5,6,6a-tetrahydro-5,5,6a-trimethyl-2(1H)-pentalenone.
 - V. Nalini and G. R. Desiraju

Acta Crystallogr., Section C, 44, 510-512 (1988).

51. The crystal and molecular structures of 4-hydroxy-3-methoxycinnamic acid, C₁₀H₁₀O₄, ferulic acid.

M. Nethaji, V. Pattabhi and G. R. Desiraju

Acta Crystallogr., Section C, 44, 275-277 (1988).

52. Prediction of non-centrosymmetric packing for 1,3-disubstituted nitro aromatics. Crystal and molecular structure of 3-hydroxy- 6-(3-nitro)-phenylazopyridine.

- G. R. Desiraju and T. S. R. Krishna Mol. Cryst. Liq. Cryst., 159, 277-287 (1988).
- Non-centrosymmetry in organic crystals: a study of molecular conformation in some substituted tolans.
 - G. R. Desiraju and T. S. R. Krishna
 - J. Chem. Soc., Chem. Commun., 192-194 (1988).
- 54. A systematic analysis of packing energies and other packing parameters for fused-ring aromatic hydrocarbons.

A. Gavezzotti and G. R. Desiraju

Acta Crystallogr., Section B, 44, 427-434 (1988).

- 55. A convenient preparation of 2,5-dibenzylidenecyclopent-3-ene-1-ones.
 - G. R. Desiraju and K. V. R. Kishan

Indian J.Chem., B27, 953-954 (1988).

- 56. Distance dependence of C- H????O interactions in some chloroalkyl compounds.
 - G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 179-180 (1989).
- 57. From molecular to crystal structure: polynuclear aromatic hydrocarbons.
 - G. R. Desiraju and A. Gavezzotti
 - J. Chem. Soc., Chem. Commun., 621-623 (1989).
- 58. Structure of 4-phenylthiazole-2(1h)-thione and 4-chlorophenacyl disulphide, the product obtained on its gas-solid chlorination.
 - V. Nalini and G. R. Desiraju

Acta Crystallogr., Section C, 45, 1525-1527 (1989).

- 59. Tautomerism in the thiazole thiones. Crystal and molecular structure of 4-(3'-nitro)-phenylthiazole-2(1H)-thione.
 - V. Nalini and G. R. Desiraju

Acta Crystallogr., Section C, 45, 1528-1530 (1989).

- 60. Crystal chemistry of some alkoxyphenylpropiolic acids. the role of oxygen and hydrogen atoms in determining stack structures of planar aromatic compounds.
 - G. R. Desiraju and K. V. R. Kishan
 - J. Am. Chem. Soc., 111, 4838-4843 (1989).
- 61. Crystal structure and solid state photoreactivity of 2,5-dibenzylidenecyclopent-3-ene-1-one and its tetrachloro derivative.
 - G. R. Desiraju, J. Bernstein, K. V. R. Kishan and J. A. R. P. Sarma Tetrahedron Lett., 30, 3029-3032 (1989).
- 62. Crystal structures of polynuclear aromatic hydrocarbons. classification, rationalisation and prediction from molecular structure.
 - G. R. Desiraju and A. Gavezzotti

Acta Crystallogr., Section B, 45, 473-482 (1989).

- 63. Solid state dimerisation of b -nitrostyrene: a disordered photoreactive crystal.
 - G. R. Desiraju and V. R. Pedireddi
 - J. Chem. Soc., Chem. Commun., 1112-1113 (1989).

- 64. Cyano????halogen interactions and their role in the crystal structures of the 4-halobenzonitriles.
 - G. R. Desiraju and R. L. Harlow
 - J. Am. Chem. Soc., 111, 6757-6764 (1989).
- 65. The nature of halogen????halogen interactions: are short halogen contacts due to specific attractive forces or due to close packing of non-spherical atoms?
 - G. R. Desiraju and R. Parthasarathy
 - J. Am. Chem. Soc., 111, 8725-8726 (1989).
- 66. Clathrate compound of a new host material: 3-hydroxy-6-(4-nitro) phenylazopyridine.
 - P. Ramachandra, T. S. R. Krishna and G. R. Desiraju

Proc. Indian Acad. Sci., (Chem. Sci.), 101, 329-334 (1989).

- 67. Strength and linearity of C- H????O bonds in molecular crystals: a database study of some terminal alkynes.
 - G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 454-455 (1990).
- 68. Structure of L-lanthionine.
 - G. R. Desiraju and D. R. Rao

Acta Crystallogr., Section C, 46, 627-629 (1990).

- 69. Structure of perhydrotriphenylene.
 - R. L. Harlow and G. R. Desiraju

Acta Crystallogr., SectionC, 46, 1054-1055 (1990).

- 70. Unexpected hydrogen bonding in the cystal structure of 4-chloro-phenylpropiolic acid. The role of C- H????O hydrogen bonds in determining O- H???O networks.
 - G. R. Desiraju, B. N. Murty and K. V. R. Kishan

Chem. Mater., 2, 447-449 (1990).

- 71. Organic compounds and materials science.
 - G. R. Desiraju

Curr. Sci. (India), 59, 452-455 (1990).

- 72. Database analysis of crystal structure determining interactions involving sulphur. Implications for the design of organic metals.
 - G. R. Desiraju and V. Nalini
 - J. Mater. Chem., 1, 201-203 (1991).
- 73. Hydration in organic crystals. prediction from molecular structure.
 - G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 426-428 (1991).
- 74. Pseudo-inversion centres in the space group P and a redetermination of the crystal structure of 3,4-dimethoxycinnamic acid. a study of non-crystallographic symmetry.
 - G. R. Desiraju, J. C. Calabrese and R. L. Harlow,

Acta Crystallogr., Section B, 47, 77-86 (1991).

- 75. C- H????O hydrogen bonding and topochemistry in crystalline 3,5-dinitrocinnamic acid and its 1:1 donor-acceptor complex with 2,5-dimethoxycinnamic acid.
 - G. R. Desiraju and C. V. K. M. Sharma
 - J. Chem. Soc., Chem. Commun., 1239-1241 (1991).

76. Unusual 2 + 2 topochemical cycloadditions of 3-cyano and 4-cyanocinnamic acids. Temperature dependent solid state photochemical reactions.

M. S. K. Dhurjati, J. A. R. P. Sarma and G. R. Desiraju

J. Chem. Soc., Chem. Commun., 1702-1703 (1991).

77. The C- H????O hydrogen bond in organic crystals. What is it? G. R. Desiraju Acc.Chem.Res., 24, 290-296 (1991).

78. C- H????O interactions and the deliberate design of organic crystal structures. G. R. Desiraju

Mol. Cryst. Liq. Cryst., 211, 63-74 (1992).

- 79. Crystal engineering and solid state chemistry of some b -nitrostyrenes.
 - V. R. Pedireddi, J. A. R. P. Sarma and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 311-320 (1992).
- Molecular recognition via C- H????O hydrogen bonding. Crystal structure of the 1:1 complex
 - 4-nitrobenzoic acid 4-(N,N-dimethylamino)benzoic acid.
 - C. V. K. M. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 832-833 (1992).
- 81. A crystallographic scale of carbon acidity.
 - V. R. Pedireddi and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 988-990 (1992).
- 82. Database analysis of Au????Au interactions.
 - S. S. Pathaneni and G. R. Desiraju
 - J. Chem. Soc., Dalton Transac., 319-322 (1993).
- 83. Structure of (4-bromophenyl)propiolic acid and its unusual hydrogen bonding pattern.

B. S. Goud and G. R. Desiraju

Acta Crystallogr., Section C, 49, 292-294 (1993).

- Structure of 4-iodo-trans-cinnamic acid and a study of carboxyl group conformation and disorder.
 - B. S. Goud, S. S. Pathaneni and G. R. Desiraju

Acta Crystallogr., Section C, 49, 1107-1111 (1993).

- 85. C- H????O packing motifs in some cyclopenta[a]phenanthrenes.
 - G. R. Desiraju, S. Kashino, M. M. Coombs and J. P. Glusker
 - Acta Crystallogr., Section B, 49, 880-892 (1993).
- 86. Determination of the crystal structure of 4-iodo-b -nitrostyrene with the aid of packing considerations: a study of halogen????nitro interactions.
 - G. R. Desiraju, V. R. Pedireddi, J. A. R. P. Sarma and D. E. Zacharias Acta Chim. Hungarica Models in Chemistry, 130, 451-465 (1993).
- 87. Evidence for O- H????C and N- H????C hydrogen bonding in crystalline alkynes, alkenes and aromatics.
 - M. A. Viswamitra, R. Radhakrishnan, J. Bandekar and G. R. Desiraju
 - J. Am. Chem. Soc., 115, 4868-4869 (1993).

- 88. Molecular tapes based on C? N????Cl interactions.
 - D. S. Reddy, K. Panneerselvam, T. Pilati and G. R. Desiraju.
 - J. Chem. Soc., Chem. Commun., 661-662 (1993).
- 89. C- H????N mediated hexagonal network in the crystal structure of the 1:1 molecular complex 1,3,5-tricyanobenzene hexamethylbenzene.
 - D. S. Reddy, B. S.Goud, K. Panneerselvam and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 663-664 (1993).
- 90. Database studies of halide ion pairs with bridging H2O and NH2 amino molecules.
 - S. S. Pathaneni and G. R. Desiraju
 - J. Chem. Soc., Dalton Transac., 2505-2508 (1993).
- 91. Solid state supramolecular assembly via C- H????O hydrogen bonds: crystal structures of the complex of 1,3,5-trinitrobenzene with dibenzylideneacetone and 2,5-dibenzylidenecyclopentanone.
 - K. Biradha, C. V. K. M. Sharma, K. Panneerselvam, L. Shimoni, H. L. Carrell, D. E. Zacharias and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 1473-1475 (1993).
- 92. Molecular recognition involving an interplay of O- H????O, C- H????O and p????p interactions. The anomalous crystal structure of the 1:1 complex 3,5-dinitrobenzoic acid 4-(N,N-dimethylamino)benzoic acid.
 - C. V. K. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 2209-2216 (1993).
- 93. N????Br mediated diamondoid network in the crystalline complex, carbon tetrabromide:hexamethylenetetramine.
 - D. S. Reddy, D. C. Craig, A. D. Rae and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 1737-1738 (1993).
- 94. Molecular and crystal structure of 1-(8-carboxyoctyl)-1,3,5,7-tetraazaadamantan-1-ium bromide and 1-(6-bromohexyl)-1,3,5,7-tetraazaadamantan-1-ium bromide.
 - D. S. Reddy, K. Panneerselvam, L. Shimoni, H. L. Carrell and G. R. Desiraju
 - J. Mol. Str., 327, 113-120 (1994).
- 95. 3-(3,5-Dinitrophenyl)-4-(2,5-dimethoxyphenyl)cyclobutane-1,2-dicarboxylic acid. Engineered topochemical synthesis, molecular and supramolecular properties.
 - C. V. K. Sharma, K. Panneerselvam, L. Shimoni, H. Katz, H. L. Carrell and G. R. Desiraju Chem. Mater., 6, 1282-1292 (1994).
- 96. Organic alloys. Diamondoid networks in crystalline complexes of 1,3,5,7-tetrabromoadamantane, hexamethylenetetramine and carbon tetrabromide.
 - D. S. Reddy, D. C. Craig and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 1457-1458 (1994).
- 97. C- H????O hydrogen bond patterns in crystalline nitro compounds. Studies in solid state molecular recognition.
 - C. V. K. Sharma and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 2345-2352 (1994).
- 98. The nature of halogen????halogen interactions and the crystal structure of 1,3,5,7-tetraiodoadamantane.
 - V. R. Pedireddi, D. S. Reddy, B. S. Goud, D. C. Craig, A.D.Rae and G. R. Desiraju

- J. Chem. Soc., Perkin Transac. 2, 2353-2360 (1994).
- 99. Towards inorganic supramolecular chemistry.

G. R. Desiraju

Proc. Indian Acad. Sci. (Chem. Sci.), 106, 593-597 (1994).

- 100. Hydrogen bonding in organometallic crystals 1. From carboxylic acids and alcohols to carbonyl compounds.
 - D. Braga, F. Grepioni, P. Sabatino and G. R. Desiraju Organometallics, 13, 3532-3543 (1994).
- 101. Molecular recognition via iodo????nitro and iodo????cyano interactions: crystal structures of the 1:1 complexes of 1,4-diiodobenzene with 1,4-dinitrobenzene and 7,7,8,8-tetracyanoquinodimethane (TCNQ).
 - F. H. Allen, B. S. Goud, V. J. Hoy, J. A. K. Howard and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 2729-2730 (1994).
- 102. Intramolecular Michael-type addition in the solid state.
 - B. S. Goud, K. Panneerselvam, D. E. Zacharias and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 325-330 (1995).
- 103. Topological equivalences between organic and inorganic crystal structures: 1,3,5,7-tetrahydroxyadamantane and caesium chloride.
 - D. S. Reddy, D. C. Craig and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 339-340 (1995).
- 104. Hexagonal supramolecular networks in the crystal structure of the 1:1 molecular complex trimethylisocyanurate 1,3,5-trinitrobenzene.
 - V. R. Thalladi, K. Panneerselvam, C. J. Carrell, H. L. Carrell and G. R. Desiraju
 - J. Chem. Soc., Chem. Commun., 340-341 (1995).
- 105. Hydrogen bonding in organometallic crystals 2. C- H????O hydrogen bonds in bridged and terminal first row metal carbonyls.
 - D. Braga, F. Grepioni, K. Biradha, V. R. Pedireddi and G. R. Desiraju
 - J. Am. Chem. Soc., 117, 3156-3166 (1995).
- 4,6-Dimethyl-2-(4-nitrobenzylidene)-3(2H)-benzofuranone.
 S. Goud, K. Panneerselvam, D. E. Zacharias and G. R. Desiraju Acta Crystallogr., Section C, 51, 265-267 (1995).
- 107. 1:1 Molecular complex of 2,3,4,5,6-pentafluoro-trans-cinnamic acid and 4-(N,N-dimethylamino)-trans-cinnamic acid.
 - B. S. Goud, P. K. Reddy, K. Panneerselvam and G. R. Desiraju Acta Crystallogr., Section C, 51, 683-685 (1995).
- 108. Methyl 3,5-dinitro-trans-cinnamate.
 - C. V. K. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju Acta Crystallogr., Section C, 51, 1364-1366 (1995).
- Supramolecular synthons in crystal engineering a new organic synthesis.
 R. Desiraju
 - Angew. Chem., 107, 2541-2557 (1995); Angew. Chem. Int. Ed. Engl., 34, 2311-2327 (1995).

- Solid state nuclear bromination of some phenols by N-bromosuccinimide.
 B. S. Goud and G. R. Desiraju
 J.Chem.Res.(S), 244-245 (1995).
- 111. (4-Dimethylaminopyridine)5(benzoic acid)3(H2O)10- a two-dimensional clathrate hydrate. K. Biradha, R. E. Edwards, G. J. Foulds, W. T. Robinson and G. R. Desiraju J. Chem. Soc., Chem. Commun., 1705-1707 (1995).
- 112. 1,3,5-Tricyanobenzene.
 D. S. Reddy, K. Panneerselvam, G. R. Desiraju, C. J. Carrell and H. L. Carrell.
 Acta Crystallogr., Section C, 51, 2352-2354 (1995).
- 113. The supramolecular concept as a bridge between organic, inorganic and organometallic crystal chemistry.
 G. R. Desiraju
 J. Mol. Str., 374, 191-198 (1996).
- 114. Hydrogen bonding in organometallic crystals 3. Transition metal complexes containing amido groups.
 K. Biradha, G. R. Desiraju, D. Braga and F. Grepioni.
 Organometallics, 15, 1284-1295 (1996).
- Supramolecular synthons in crystal engineering. Structure simplification, synthon robustness and supramolecular retrosynthesis.
 V. R. Thalladi, B. S. Goud, V. J. Hoy, F. H. Allen, J. A. K. Howard and G. R. Desiraju Chem.Comm., 401-402 (1996).
- 116. First neutron diffraction analysis of an O- H????p hydrogen bond. 2-Ethynyladamantan-2-ol F. H. Allen, J. A. K. Howard, V. J. Hoy, G. R. Desiraju, D. S. Reddy and C.C.Wilson J. Am. Chem. Soc., 118, 4081-4084 (1996).
- 117. Supramolecular synthons in crystal engineering. 3 Solid state architecture and synthon robustness in some 2,3-dicyano-5,6-dichloro-1,4-dialkoxybenzenes.
 D. S. Reddy, Y. E. Ovchinnikov, O. V. Shishkin, Y. T. Struchkov and G. R. Desiraju J. Am. Chem. Soc., 118, 4085-4089 (1996).
- Supramolecular synthons in crystal engineering. 4 Structure simplification and synthon interchangeability in some organic diamondoid solids.
 D. S. Reddy, D. C. Craig and G. R. Desiraju
 J. Am. Chem. Soc., 118, 4090-4093 (1996).
- 119. Crystal engineering and molecular recognition twin facets of supramolecular chemistry: G. R. Desiraju and C. V. K. Sharma in The Crystal as a Supramolecular Entity Ed. G. R. Desiraju, Perspectives in Supramolecular Chemistry, 2, Wiley, Chichester, 1996, pp 31-61.
- Correlation of biological activity in b -lactam antibiotics with Woodward and Cohen structural parameters A Cambridge Database study
 A. Nangia, K. Biradha and G. R. Desiraju
 J. Chem. Soc., Perkin Transac. 2, 943-954 (1996).
- 121. Review of general principles: G. R. Desiraju in Comprehensive Supramolecular Chemistry, Eds. D. D. MacNicol, R. Bishop, F. Toda, Volume 6, "Crystal Engineering", Pergamon, New York, 1996, pp 1-22.

- 122. Organic solid state reactivity past, present and future: G. R. Desiraju and B.S.Goud in Solid State Reactivity Past, Present and Future, Ed. V. V. Boldyrev, Blackwell, Oxford, 1996, pp 223-236.
- 123. Hydrogen bonding in organometallic crystals. 4. M-H????O hydrogen-bonding interactions. D. Braga, F. Grepioni, E. Tedesco, K. Biradha and G. R. Desiraju Organometallics, 15, 2692-2699 (1996).
- Agostic interactions in organometallic compounds. A Cambridge Structural Database study.
 D. Braga, F. Grepioni, K. Biradha and G. R. Desiraju
 J. Chem. Soc., Dalton Trans., 3925-3930 (1996).
- The C- H????O hydrogen bond: structural implications and supramolecular design G. R. Desiraju Acc.Chem.Res.29, 441-449 (1996).
- 126. The hydrogen bond C- H donor and p -acceptor characteristics of three-membered rings F. H. Allen, J. P. M. Lommerse, V. J. Hoy, J. A. K. Howard and G. R. Desiraju Acta Crystallogr., Section B, 52, 734-745 (1996).
- Odd-even carbon atom disparity in organic compounds
 J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass and J. D. Dunitz Nature (London), 384, 320 (1996).
- 2,6-Dibenzoylhydroquinone
 K. Biradha, A. K. Katz, H. L. Carrell and G. R. Desiraju Acta Crystallogr., Section C, 52, 2839-2841 (1996).
- 129. Design of a SHG-active crystal, 4-iodo-4-nitrobiphenyl. The role of supramolecular synthons. J. A. R. P. Sarma, F. H. Allen, V. J. Hoy, J. A. K. Howard, R. Thaimattam, K. Biradha, and G. R. Desiraju Chem.Comm., 101-102 (1997).
- 2,4-Dinitro-trans-cinnamic acid
 V. R. Thalladi, C. V. K. Sharma and G. R. Desiraju
 Acta Crystallogr., Section C, 53, 227-229 (1997).
- 131. Crystal engineering and correspondence between molecular and crystal structures. Are 2-and 3-aminophenol anomalous?
 F. H. Allen, V. J. Hoy, J. A. K. Howard, V. R. Thalladi and G. R. Desiraju
 J. Am. Chem. Soc., 119, 3477-3480 (1997).
- 132. Hydrogen bonding in organometallic crystals. 6. X-H????M hydrogen bonds and M????(H-X) pseudo-agostic bonds
 D. Braga, F. Grepioni, E. Tedesco, K. Biradha and G. R. Desiraju
 Organometallics, 16, 1846-1856 (1997).
- 133. Even odder carbons J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass and J.D.Dunitz Nature (London), 387, 464 (1997).
- C- H????O hydrogen bonded multi-point recognition in molecular assemblies of dibenzylideneketones and 1,3,5-trinitrobenzenes.
 K. Biradha, A. Nangia, G. R. Desiraju, C. J. Carrell and H. L. Carrell

- J. Mater.Chem., 1111-1122 (1997).
- Crystal engineering: solid state supramolecular synthesis
 G. R. Desiraju
 Curr. Opin.Solid State & Materials Science, 2, 451-454 (1997).
- Designer crystals: intermolecular interactions, network structures and supramolecular synthons
 R. Desiraju Chem.Comm., 1475-1482 (1997).
- 137. Engineering of an octupolar non-linear optical crystal: tribenzyl isocyanurate V. R. Thalladi, S. Brasselet, D. Blll r, R. Boese, J. Zyss, A. Nangia and G. R. Desiraju Chem. Comm., 1841-1842 (1997).
- 138. Evidence for the characterisation of the C- H????p interaction as a weak hydrogen bond: toluene and chlorobenzene solvates of 2,3,7,8-tetraphenyl-1,9,10-anthyridine N. N. L. Madhavi, A. K. Katz, H. L. Carrell, A. Nangia and G. R. Desiraju Chem. Comm., 1953-1954 (1997).
- Crystal gazing: structure prediction and polymorphism G. R. Desiraju Science, 278, 404-405 (1997).
- 140. Reactivity of organic solids retrospect and prospectG. R. DesirajuSolid State Ionics, 101-103, 839-842 (1997).
- 2,6-Dibenzoyl-1,4-benzoquinone
 K. Biradha, M. J. Zaworotko, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 53, 1653-1655 (1997).
- 142. The halogen????O(nitro) supramolecular synthon in crystal engineering: a combined crystallographic database and ab initio molecular orbital study F. H. Allen, J. P. M. Lommerse, V. J. Hoy, J. A. K. Howard, G. R. Desiraju Acta Crystallogr., Section B, 53, 1006-1016 (1997).
- 143. Hydrogen bonding in organometallic crystals a survey D. Braga, F. Grepioni and G. R. Desiraju J. Organomet. Chem., 548, 33-43 (1997).
- 144. Molecular networks in the crystal structures of tetrakis-(4-iodophenyl)methane and (4-iodophenyl)triphenylmethane R. Thaimattam, D. S. Reddy, F. Xue, T. C. W. Mak, A. Nangia and G. R. Desiraju New J. Chem., 22, 143-148 (1998).
- 145. 4-(Triphenylmethyl) benzoic acid: a supramolecular wheel-and-axle host R. K. R. Jetti, S. S. Kuduva, D. S. Reddy, F. Xue, T. C. W. Mak, A. Nangia, G. R. Desiraju. Tetrahedron Lett., 39, 913-916 (1998).
- 146. Crystal engineering: some further strategies.
 A. Anthony, G. R. Desiraju, R. K. R.Jetti, S. S. Kuduva, N. N. L.Madhavi, A. Nangia, R. Thaimattam, V. R. Thalladi.

Crystal Engineering, 1, 1-18 (1998).

- Trimethylisocyanurate and triethylisocyanurate
 R. Thalladi, A. K. Katz, H. L. Carrell, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 54 86-89 (1998).
- 148. Crystal engineering of some 2,4,6-triaryloxy-1,3,5-triazines: octupolar non-linear materials V. R. Thalladi, S. Brasselet, H. -C. Weiss, D. Bll r, A. K. Katz, H. L. Carrell, R. Boese, J. Zyss, A. Nangia and G. R. Desiraju J. Am. Chem. Soc., 120, 2563-2577 (1998).
- Distinction between the weak hydrogen bond and the van der Waals interaction T. Steiner and G. R. Desiraju Chem. Comm., 891-892 (1998).
- Supramolecular synthons and pattern recognition
 A. Nangia and G. R. Desiraju
 Topics in Current Chemistry, "Design of Organic Solids", Vol. 198 (ed. E.Weber)
 57-95 (1998).
- Crystal engineering and organometallic architecture
 Braga, F. Grepioni and G. R. Desiraju,
 Chem. Rev., 98, 1375-1405 (1998).
- 152. Octupolar versus dipolar crystalline structures for nonlinear optics: a dual crystalline and propogative engineering approach
 - J. Zyss, S. Brasselet, V. R. Thalladi, G. R. Desiraju
 - J. Chem. Phys. 109, 658-669 (1998)
- 153. Interplay of strong and weak hydrogen bonding in molecular complexes of some 4,4-disubstituted biphenyls with urea, thiourea and water R. Thaimattam, D. S. Reddy, F. Xue, T. C. W.Mak, A. Nangia and G. R. Desiraju
 - J. Chem. Soc., Perkin Transac. 2, 1783-1789 (1998).
- 154. Synthesis, X-ray crystal structures and biological evaluation of some mono- and bicyclic 1,3diazetidin-2-ones
 - P. S. Chandrakala, A. K. Katz, H. L. Carrell, P. R. Sailaja, A. R. Podile, A. Nangia and G. R. Desiraju,
 - J. Chem. Soc., Perkin Transac. 1, 2597-2609 (1998).
- C- H????F interactions in the crystal structures of some fluorobenzenes
 R. Thalladi, H. -C.Weiss, D. Bll r, R. Boese, A. Nangia and G. R. Desiraju
 J. Am. Chem. Soc., 120, 8702-8710 (1998).
- 156. Isostructurality in crystalline oxa-androgens. A case of C- O- H???O and C- H????O interaction mimicry and solid solution formation.
 A. Anthony, M. Jask□ i, A. Nangia and G. R. Desiraju Chem. Comm., 2537-2538 (1998).
- Supramolecular structures reason and imagination
 A. Nangia and G. R. Desiraju
 Acta Crystallogr., Section A, 54, 934-944 (1998).

158. Supramolecular synthons mediated by weak hydrogen bonding. Forming linear molecular arrays via C? C- H????N? C and C? C- H????O₂N recognition.

R. Thaimattam, P. J. Langley, J. Hulliger and G. R. Desiraju New J. Chem. 1307-1309 (1998).

159. 17,17-Ethylenedioxyandrost-4-ene-3,6-dione and 17,17-ethylenedioxyandrosta- 1,4-diene-3,6-dione

A. Anthony, M. Jask□i, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 54 1894-1898 (1998).

160. 5b -Androstan-3,17-dione

A. Anthony, M. Jask i, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 54 1898-1900 (1998).

161. Some current challenges in crystal engineering

A. Nangia and G. R.Desiraju, in Supramolecular Engineering of Synthetic Metallic Materials: Conductors and Magnets, Eds. J. Veciana, C. Rovira, D.B. Amabilino, NATO ASI Series, Kluwer, Dordrecht, 1999, pp 1-21.

162. Weak hydrogen bonds in supramolecular synthesis

A. Nangia and G. R.Desiraju, in Current Challenges on Large Supramolecular Assemblies, Ed. G. Tsoucaris, NATO ARW Series, Kluwer, Dordrecht, 1999, pp 193-208.

163. Axial and equatorial conformations of penicillins, their sulfoxides and sulfones: The role of N-H????S and C-H????O hydrogen bonds

A. Nangia and G. R. Desiraju

J. Mol. Str., 474, 65-79 (1999).

164. Cubane carboxylic acids. Crystal engineering considerations and the role of C- H????O hydrogen bonds in determining O-H????O networks

S. S. Kuduva, D. C. Craig, A. Nangia and G. R. Desiraju

J. Am. Chem. Soc., 121, 1936-1944 (1999).

Crystal structure of sodium glutaconaldehyde tetrahydrate, Na2(C5H5O2)2. 4H2O
 M. Muthuraman, Y. le Fur, J. -F. Nicoud, R. Masse and G. R. Desiraju
 Z. Kristallogr. NCS, 214, 283-284 (1999).

166. Pseudopolymorphism. Occurrences of hydrogen bonding organic solvents in molecular crystals

A. Nangia and G. R. Desiraiu

Chem. Comm., 605-606 (1999).

167. Tri-p-tolyl-1,3,5-triazine

V. R. Thalladi, M. Muthuraman, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 55 698-700 (1999).

168. Pseudopolymorphs of 3,5-dinitrosalicylic acid

V. R. Senthil Kumar, S. S. Kuduva and G. R. Desiraju

J. Chem. Soc., Perkin Transac. 2, 1069-1073 (1999).

169. Current challenges in crystal engineering

G. R. Desiraju, in Implications of Molecular and Materials Structure for New Technologies, Eds. J. A. K. Howard, F. H. Allen and G. P. Shields, Kluwer, Dordrecht, 1999, pp 321-339.

- 170. Steering non-centrosymmetry into the third dimension. Crystal engineering of an octupolar nonlinear optical crystal. V. R. Thalladi, R. Boese, S. Brasselet, I. Ledoux, J. Zyss, R. K. R. Jetti and G. R. Desiraju Chem. Comm., 1639-1640 (1999).
- 171. When is a polymorph not a polymorph? Helical trimeric O-H????O synthons in trans-1,4diethynyl-1,4-cyclohexanediol. C. Bilton, J. A. K. Howard, N. N. L. Madhavi, A. Nangia, G. R. Desiraju and F. H. Allen Chem. Comm., 1675-1676 (1999).
- 172. Sodium 4-nitrophenolate 4-nitrophenol dihydrate crystal: a new herringbone structure for quadratic nonlinear optics M. Muthuraman, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud and G. R. Desiraju J. Mater. Chem, 1471-1474 (1999).
- 173. Engineering of nonlinear optical crystals displaying a quasi perfect polar alignment of chromophores M. Muthuraman, Y. LeFur, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud and G. R. Desiraju J. Mater. Chem, 2233-2239 (1999).
- 174. 4-(Triphenylmethyl)phenol-Triphenylphosphine oxide (1/1) R.K.R.Jetti, H.-C.Weiss, V. R. Thalladi, R. Boese, A. Nangia and G. R. Desiraju Acta Crystallogr., Section C, 55, 1530-1533 (1999).
- 175. Polymorphism and Pseudopolymorphism in Organic Crystals. A Cambridge Structural Database Study J. A. R. P. Sarma and G. R.Desiraju, in Crystal Engineering. The Design and Applications of Functional Solids, Eds. K.R.Seddon and M.Zaworotko, Kluwer, Dordrecht, 1999, pp 325-
- 176. Diversity and certainty Database research in crystal engineering G. R. Desiraju, in Crystal Engineering: From molecules and crystals to materials, Eds. D. Braga et al., Kluwer, Dordrecht, 1999, pp 229-241.
- 177. The indecisive role of the C-F group in crystal packing-an analysis of the crystal structures of the tetrahalogenated hydroquinones and g -hydroquinone V. R. Thalladi, H.-C.Weiss, R. Boese, A. Nangia and G. R. Desiraju Acta Crystallogr., Section B, 55 1005-1013 (1999).
- 178. The even/odd disparity in organic compounds G. R. Desiraju, J. D. Dunitz, A. Nangia, J. A. R. P. Sarma and E. Zass Helv. Chim. Acta, 83, 1-15 (2000).
- 179. Establishing structural repetitivity in systems with interaction interference: crystal engineering in the gem-alkynol family N. N. L. Madhavi, C. Bilton, J. A. K. Howard, F. H. Allen, A. Nangia and G. R. Desiraju New J. Chem., 24, 1-4 (2000).
- 180. Molecular dynamics study of the solid state photoreactivity of 3- and 4-cyano-trans-cinnamic J. A. R. P. Sarma, B. Chaudhuri and G. R. Desiraju

- C-H????O and C-H????N hydrogen bond networks in the crystal structures of some 1,2-dihydro-N-aryl-4,6-dimethylpyrimidin-2-ones
 M. Muthuraman, Y. LeFur, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud, S. George, A. Nangia and G. R. Desiraju
 J. Solid State Chem., 152, 221-228 (2000).
- 182. The supramolecular synthon in crystal engineering G. R. Desiraju in, Stimulating concepts in chemistry, Eds. S. Shibasaki, J. F. Stoddart, F. V?e, Wiley, Chichester, 2000, pp. 293-308.
- 183. Tris-(2-Cyanoethyl)isocyanurate
 P. K. Thallapally and G. R.Desiraju
 Acta Crystallogr., Section C, 56, 572-573 (2000).
- 184. Three dimensional Quantitative Structural Activity Relation (3D QSAR) studies of some 1,5-diarylpyrazoles: Analogue based design of selective cyclooxygenase-2 inhibitors. G. R. Desiraju, B. Gopalakrishnan, R. K. R. Jetti, D. Raveendra, J. A. R. P. Sarma and H. S. Subramanya Molecules, 5, 945-955 (2000).
- 185. Shape and size effects in the crystal structures of complexes of 1,3,5-trinitrobenzene with some trigonal donors: the benzene-thiophene exchange rule.
 P. K. Thallapally, K. Chakraborty, H. L. Carrell, S. Kotha and G. R. Desiraju Tetrahedron, 56, 6721-6728 (2000).
- 186. Benzyltriphenylphosphonium glutaconaldehyde M. Muthuraman, J. -F. Nicoud, R. Masse and G. R. Desiraju Acta Crystallogr., Section C, 56, 986-988 (2000).
- 187. Hydrogen bonding and other intermolecular interactions in organometallic crystals G. R. Desiraju J. Chem. Soc., Dalton Transac., 3745-3752 (2000).
- 188. Melting points of meta and para isomers of 4-anisylpinacolone S. S. Kuduva, J. A. R. P. Sarma, A. K. Katz, H. L. Carrell and G. R. Desiraju J. Phys. Org. Chem. 13, 719-728, (2000).
- 4-Ethynyl-4-hydroxy-cyclohexanone and 4-ethynyl-4-hydroxy-2,3,4,5-tetramethylcyclohexa-2,5-diene-1-one
 Bilton, J. A. K. Howard, N. N. L. Madhavi, G. R. Desiraju and F. H. Allen Acta Crystallogr., Section C, 56, 1356-1358 (2000).
- 190. Racemic 1,2-diphenyl-3-butyn-2-ol N. N. L. Madhavi, G. R. Desiraju, C. Bilton, J. A. K. Howard and F. H. Allen Acta Crystallogr., Section C, 56, 1359-1360 (2000).
- Crystal engineering in the gem-alkynol family: interplay between strong and weak interactions in structures of 2,3,5,6-tetrahalo[F,Cl,Br]-trans-1,4-diethynyl-cyclohexa-2,5-diene-1,4-diols
 N. N. L. Madhavi, G. R. Desiraju, C. Bilton, J. A. K. Howard and F. H. Allen Acta Crystallogr., Section B, 56, 1063-1070, (2000).
- 192. Crystal engineering in the gem-alkynol family: synthon repetitivity and topological similarity in diphenylethynylmethanols: structures that lack O-H????O hydrogen bonds

C. Bilton, J. A. K. Howard, N. N. L. Madhavi, A. Nangia, G. R. Desiraju, F. H. Allen and C. C. Wilson

Acta Crystallogr., Section B, 56, 1071-1079, (2000).

Acta Crystallogr., Section B, 56, 1080-1084, (2000).

193. Halogen trimer synthons in crystal engineering: low temperature X-ray and neutron diffraction study of the 1:1 complex of 2,4,6-tris(4-chlorophenoxy)-1,3,5-triazine with tribromobenzene
C. K. Broder, J. A. K. Howard, D. A. Keen, C. C. Wilson, F. H. Allen, R. K. R. Jetti, A. Nangia and G. R. Desiraju

194. The All-Chemist (Millennium Essay)

G. R. Desiraju

Nature (London), 408, 407 (2000).

195. Crystallisation of pseudopolymorphs of some gamboge pigments. Pyridine, dimethylformamide and dimethylsulfoxide solvates of morellic acid, gambogic acid and guttiferic acid.

A. Anthony and G. R. Desiraju

Supramolecular Chemistry, 13, 11-23 (2001).

196. Hydrogen bonding in two tetracyclic indole alkaloids A. K. Varma, A. Nangia, G. R. Desiraju, V. S. Giri and P. Jaisankar Acta Crystallogr., Section C, 57, 97-99 (2001).

- 197. Crystal engineering of primary cubanecarboxamides. Repetitive formation of an unexpected N-H...O hydrogen bonded network
 - S. S. Kuduva, D. Bll r, R. Boese and G. R. Desiraju

J. Org. Chem., 66, 1621-1626 (2001).

Diamond and square grid networks in the same structure. Crystal engineering with the iodo????nitro supramolecular synthon.
 R. Thaimattam, C. V. K. M. Sharma, A. Clearfield and G. R. Desiraju Cryst. Growth & Des., 1, 103-106 (2001).

Nonlinear optical crystals designed with 4-nitrophenolate chromophores: An engineering route using a multipdipolar chromophore, 3-hydroxy-2,4,6-trinitrophenolate.
 M. Muthuraman, J. ?F. Nicoud, R. Masse and G. R. Desiraju Mol. Cryst. Liq. Cryst., 356, 1-13 (2001).

Area correction of multiatom acceptor hydrogen bond frequency distributions.
 Ciunik and G. R. Desiraju
 Chem. Comm., 703-704 (2001).

201. Molecular Complexation as a design tool in the crystal engineering of non-centrosymmetric structures. Ideal orientation of chromophores linked by O?H???O and C?H???O hydrogen bonds for nonlinear optics
M. Muthuraman, R. Masse, J. ?F. Nicoud and G. R. Desiraju
Chem. Mater., 13, 1473-1479 (2001).

202. Inclusion compounds of tetrakis-(4-nitrophenyl)methane: C?H???O networks, pseudopolymorphism and structural transformations R. Thaimattam, X. Feng, J. A. R. P. Sarma, T. C. W. Mak and G. R. Desiraju J. Am. Chem. Soc., 123, 4432-4445 (2001).

- 203. Crystal structures and packing of 4-cyanocubane carboxylic acid, its ethyl ester and the solid solution of 1,4-dicyanocubane and 1,4-dibromocubane
 S. S. Kuduva, D. Bll r, R. Boese and G. R. Desiraju
 Structural Chemistry, 12, 259-266 (2001).
- 204. Matching of molecular and supramolecular symmetry. An exercise in crystal engineering. P. K. Thallapally, K. Chakraborty, A. K. Katz, H. L. Carrell, S. Kotha and G. R. Desiraju CrystEngComm, 31, (2001).
- Chemistry beyond the molecule
 G. R. Desiraju,
 Nature (London), 412, 397-400 (2001).
- 206. Computer aided design of selective COX-2 inhibitors: comparative molecular field analysis and docking studies of some 3,4-diaryloxazolone derivatives
 G. R. Desiraju, J. A. R. P. Sarma, D. Raveendra, B. Gopalakrishnan, R. Thilagavathi, M. E. Sobhia and H. S. Subramanya
 J. Phys. Org. Chem., 14, 481-487 (2001).
- 207. Crystal engineering in the gem-alkynol family. The key role of water in the structure of 2,3,5,6-tetrabromo-trans-1,4-diethynyl-cyclohexa-2,5-diene-1,4-diol monohydrate C. Bilton, J. A. K. Howard, N. N. L. Madhavi, G. R. Desiraju, F. H. Allen, D. A. Keen and C. C. Wilson Acta Crystallogr., Section B, 57, 560-566 (2001).
- Crystal structure of N,N?-di-5-nitrosalicylidene-(R,R)-1,2-cyclohexanediamine, C20H20N4O6
 M. Muthuraman, J. ?F. Nicoud, R. Masse and G. R. Desiraju
 Z. Kristallogr. NCS, 216, 381-382 (2001).
- 209. Crystal structure of N,N?-di-5-nitrosalicylidene-(R,S)-1,2-cyclohexanediamine, C20H20N4O6
 M. Muthuraman, J. ?F. Nicoud, R. Masse and G. R. Desiraju
 Z. Kristallogr. NCS, 216, 383-384 (2001).
- Crystal engineering. Outlook and prospects.
 G. R. Desiraju
 Curr. Sci., 81, 1038-1042 (2001).
- 211. Steroidal aromatase inhibitors. Model receptor surfaces and 3D QSAR. R. K. R. Jetti, A. Anthony, A. Nangia and G. R. Desiraju Ind. J. Chem. Section B, 40, 1054-1062 (2001).
- Unusually long cooperative chain of seven hydrogen bonds. An alternative packing type for symmetrical phenols.
 P. K. Thallapally, A. K. Katz, H. L. Carrell and G. R. Desiraju Chem. Comm. 344-345 (2002).
- 213. 3D-QSAR Studies of some [[1-Aryl(or Benzyl)-1-(benzenesulphonamido)methyl] phenyl] alkanoic acid derivatives as Thromboxane A2 Receptor Antagonists K. V. V. M. Sairam, J. A. R. P. Sarma and G. R. Desiraju Drug Design and Discovery, 18, 45-49 (2002).

- 214. Topological Equivalences between Organic and Coordination Polymer Crystal Structures: An organic ladder formed with three?connected molecular and supramolecular synthons S. Aitipamula, P. K. Thallapally, R. Thaimattam, M. Jaskolski and G. R. Desiraju Org. Lett., 4, 921-924 (2002).
- 215. The supramolecular synthon approach to crystal structure prediction J. A. R. P. Sarma and G. R. Desiraju Cryst. Growth Des., 2, 93-100 (2002).
- 1,3-Dibromo-2,4,6-trinitrobenzene (DBTNB). Crystal engineering and perfect polar alignment of two-dimensional hyperpolarizable chromophores
 P. K. Thallapally, G. R. Desiraju, M. Bagieu-Beucher, R. Masse, C. Bourgogne and J. F. Nicoud
 Chem. Comm., 1052-1053 (2002).
- 217. Hydrogen bridges in crystal engineering. Interactions without borders. G. R. Desiraju Acc. Chem. Res., 35, 565-573 (2002).
- 218. Supramolecular synthons based on N?HnII and C?HnII hydrogen bonds. Crystal engineering of a helical structure with 5,5-diethylbarbituric acid. P. Vishweshwar, R. Thaimattam, M. Jaskolski and G. R. Desiraju Chem. Comm. 1830-1831 (2002).
- 219. Crystallography. Quo vadis?G. R. DesirajuZ. Krist., 217, 297-298 (2002).
- 220. ?Bond free?.G. R. DesirajuCrystEngComm, 4, 499 (2002).
- Innovation in crystal engineering
 Braga, G. R. Desiraju, J. S. Miller, A. G. Orpen and S. L. Price CrystEngComm, 4, 500-509 (2002).
- 222. Crystal structures and packing of 2,4,6-tris(4-fluorophenoxy)-1,3,5-triazine and 2,4,6-tris(3,4-dimethylphenoxy)-1,3,5-triazine. New materials for octupolar nonlinear optics.
 R. Boese, G. R. Desiraju, R. K. R. Jetti, M. T. Kirchner, I. Ledoux, V. R. Thalladi, and J. Zyss Struct. Chem. 13, 321-328 (2002).
- Cryptic crystallography
 G. R. Desiraju
 Nature Materials, 1, 77-79 (2002).
- 224. A 1:1 molecular complex of bis(4-aminophenyl)disulfide and 4-aminothiophenol V. R. Vangala, G. R. Desiraju, R. K. R. Jetti, D. Bill r and R. Boese Acta Crystallogr., Section C, 58, o635-o636 (2002).
- 3,5-Dinitrosalicylic acid?phenazine (1/1)
 V. S. Senthil Kumar, S. S. Kuduva and G. R. Desiraju Acta Crystallogr., Section E, 58, o865-o866 (2002).

226. Computer aided design of selective COX-2 inhibitors: Comparative Molecular Field Analysis (CoMFA), Comparative Similarity Indices Analysis (CoMSIA) and docking studies of some 1,2-diarylimidazole derivatives.

G. R. Desiraju, B. Gopalakrishnan, R. K. R. Jetti, A. Nagaraju, D. Raveendra,

J. A. R. P. Sarma, M. E. Sobhia and R. Thilagavathi,

J. Med. Chem. 45, 4847-4857 (2002).

227. Database study of N-H...O, O-H...O and C-H...O hydrogen bonds in protein-ligand complexes

S. Sarkhel and G. R. Desiraju

Protein: Structure, Function and Bioinformatics, 54, 247-259 (2004).

228. Polymorphism of 1,3,5-trinitrobenzene induced by trisindane additive P. K. Thallapally, R. K. R. Jetti, A. K. Katz, H. L. Carrell, K. Singh, K. Lahiri, S. Kotha, R. Boese, G. R. Desiraju Angew Chem. Int. Ed., 43, 1149-1155 (2004).

- 229. Gauche and staggered forms of diethylamine in solvates of 1,5-dichloro-cis-9,10-diethynyl-9,10-dihydroanthracene-9,10-diol. A case of conformational pseudopolymorphism? R. Mondal, J. A. K. Howard, R. Banerjee and G. R. Desiraju Chem. Comm., 644-645 (2004).
- Homology modelling in protein in protein structure prediction: Epidermal Growth Factor Receptor kinase domain
 K. Panigrahi and G. R. Desiraju
 Natnl. Acad. Sci. Lett., 27 1-12 (2004).
- 231. Host-guest and network structures of some tetraphenylmethane derivatives S. Basavoju, S. Aitipamula, G. R. Desiraju CrystEngComm., 6, 642-646 (2004).
- 232. A 1:1 molecular complex of 4-aminocyclohexanol and (4-hydroxycyclohexyl)- carbamic acid A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard Acta Crystallogr., Sect. E, 60, o857-o859 (2004).
- 233. Hydrogen Bonding G. R. Desiraju

Ency. Supr. Chem. (Eds. J. L. Atwood and J. Steed) Marcel Dekker, New York, 2004, 1, pp 658-665.

Organic chlorine as a hydrogen bridge acceptor. Evidence for the existence of intramolecular O?H?CI?C interactions in some gem-alkynols.
 R. Banerjee, G. R. Desiraju, R. Mondal, J. A. K. Howard Chem. Eur. J. 10, 3373-3383 (2004).

- 235. A novel saturated hydrogen bridge architecture in supraminols B. R. Bhogala, V. R. Vangala, P. S. Smith, J. A. K. Howard, G. R. Desiraju Cryst. Growth & Des., 4, 647-649 (2004).
- Structural variations and polymorphism of some derivatives of 6-amino-2-phenylsulfonylimino-1,2-dihydropyridine
 M. T. Kirchner, L. S. Reddy, G. R. Desiraju, R. K. R. Jetti, R. Boese Cryst. Growth & Des., 4, 701-709 (2004).

237. Midsummer madness (Turning Point Essay)

G. R. Desiraju

Nature, 431, 25 (2004).

238. Proton transfer and N(+)?H...S(?) hydrogen bonds in the crystal structure of 4-aminothiophenol

R. K. R. Jetti, R. Boese, T. S. Thakur, V. R. Vangala, G. R. Desiraju Chem. Comm., 2526-2527 (2004).

239. Crystal engineering in the aminophenol family. Novel carborundum network in a supramolecular homologous series.

A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard Chem. Comm., 2528-2529 (2004).

240. Counterpoint: What's in a name?

G. R. Desiraju

Cryst. Growth & Des., 4, 1089-1090 (2004).

241. Supramolecular equivalence of ethynyl, chloro, bromo and iodo groups. A comparison of the crystal structures of some 4-phenoxyanilines.

A. Dey and G. R. Desiraju

CrystEngComm., 6, 642-646 (2004).

242. Database study of N-H...O, O-H...O and C-H...O hydrogen bonds in protein-ligand complexes

S. Sarkhel and G. R. Desiraiu

Protein: Structure, Function and Bioinformatics, 54, 247-259 (2004).

243. Polymorphism of 1,3,5-trinitrobenzene induced by trisindane additive

P. K. Thallapally, R. K. R. Jetti, A. K. Katz, H. L. Carrell, K. Singh, K. Lahiri, S. Kotha, R. Boese, G. R. Desiraiu

Angew Chem. Int. Ed., 43, 1149-1155 (2004).

244. Gauche and staggered forms of diethylamine in solvates of 1,5-dichloro-cis-9,10-diethynyl-9,10-dihydroanthracene-9,10-diol. A case of conformational pseudopolymorphism?
R. Mondal, J. A. K. Howard, R. Banerjee and G. R. Desiraju
Chem. Comm., 644-645 (2004).

245. Homology modelling in protein in protein structure prediction: Epidermal Growth Factor Receptor kinase domain

S. K. Panigrahi and G. R. Desiraju

Natnl. Acad. Sci. Lett., 27 1-12 (2004).

246. Host-guest and network structures of some tetraphenylmethane derivatives S. Basavoju, S. Aitipamula, G. R. Desiraju CrystEngComm., 6, 642-646 (2004).

247. A 1:1 molecular complex of 4-aminocyclohexanol and (4-hydroxycyclohexyl)- carbamic acid A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard Acta Crystallogr., Sect. E, 60, o857-o859 (2004).

248. Hydrogen Bonding

G. R. Desiraju

Ency. Supr. Chem. (Eds. J. L. Atwood and J. Steed) Marcel Dekker, New York, 2004, 1, pp.

658-665.

- Organic chlorine as a hydrogen bridge acceptor. Evidence for the existence of intramolecular O?H?CI?C interactions in some gem-alkynols.
 R. Banerjee, G. R. Desiraju, R. Mondal, J. A. K. Howard Chem. Eur. J. 10, 3373-3383 (2004).
- A novel saturated hydrogen bridge architecture in supraminols
 B. R. Bhogala, V. R. Vangala, P. S. Smith, J. A. K. Howard, G. R. Desiraju
 Cryst. Growth & Des., 4, 647-649 (2004).
- Structural variations and polymorphism of some derivatives of 6-amino-2-phenylsulfonylimino-1,2-dihydropyridine
 M. T. Kirchner, L. S. Reddy, G. R. Desiraju, R. K. R. Jetti, R. Boese Cryst. Growth & Des., 4, 701-709 (2004).
- 252. Midsummer madness (Turning Point Essay) G. R. Desiraju Nature,431,25 (2004).
- Proton transfer and N(+)?H...S(?) hydrogen bonds in the crystal structure of 4-aminothiophenol
 R. K. R. Jetti, R. Boese, T. S. Thakur, V. R. Vangala, G. R. Desiraju
 Chem. Comm., 2526-2527 (2004).
- 254. Crystal engineering in the aminophenol family. Novel carborundum network in a supramolecular homologous series.
 A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard Chem. Comm., 2528-2529 (2004).
- 255. Counterpoint: What's in a name?
 G. R. Desiraju
 Cryst. Growth & Des., 4, 1089-1090 (2004).
- 256. Supramolecular equivalence of ethynyl, chloro, bromo and iodo groups. A comparison of the crystal structures of some 4-phenoxyanilines.
 A. Dey and G. R. Desiraju
 CrystEngComm., 6, 642-646 (2004).
- 257. Dianiline diphenol molecular complexes based on supraminol recognition. V. R. Vangala, R. Mondal, C. K. Broder, J. A. K. Howard, G. R. Desiraju Cryst. Growth & Des., 5, 99-104 (2005).
- Chemistry. The Middle Kingdom.
 G. R. Desiraju
 Curr. Sci., 88, 374-380 (2005).
- Saccharin as a salt former. Enhanced solubilities of saccharinates of active pharmaceutical ingredients.
 P. M. Bhatt, N. V. Ravindra, R. Banerjee and G. R. Desiraju Chem. Comm., 1073-1075 (2005).
- 260. Structural studies of the system (Na⁺)(saccharinate[?])(H2O)n. A model for crystallization. R. Banerjee, P. M. Bhatt, M. T. Kirchner and G. R. Desiraju

Angew. Chem. Int. Ed., 44, 2515-2520 (2005). (VIP)

261. 2-Methylsulfanylnicotinic acid.

S. Basavoju, C. M. Reddy and G. R. Desiraju Acta Crystallogr., Sect. E, 61, 0822-0833 (2005).

262. Virtual Screening of 4-Anilinoquinazoline Analogs as EGFR Kinase Inhibitors: Importance of Hydrogen Bonds in the Evaluation of Poses and Scoring Functions.

V. Aparna, G. Rambabu, S. K. Panigrahi, J. A. R. P. Sarma and G. R. Desiraju

J. Chem. Inf. Model., 45, 725-738 (2005).

263. Sorting of polymorphs based on mechanical properties. Trimorphs of 6-chloro- 2,4-dinitroaniline.

C. M. Reddy, S. Basavoju and G. R. Desiraju

Chem. Comm., 2439-2441 (2005).

264. Correlation between molecular dipole moment and centrosymmetry in some crystalline diphenyl ethers.

A. Dey and G. R. Desiraju

Chem. Comm., 2486-2488 (2005).

265. A rare syn?anti catemer in 4-nitrophenylpropiolic acid.

D. Das, G. R. Desiraju, R. K. R. Jetti and R. Boese

Acta Crystallogr., E, 61, 01588? 01589 (2005).

266. A virtual screening approach for thymidine monophosphate kinase inhibitors as antitubercular agents based on docking and pharmacophore models.

B. Gopalakrishnan, V. Aparna, J. Jeevan, M. Ravi and G. R. Desiraju

J. Chem. Inf. Model., 45, 1101-1108 (2005).

267. C?H?O and other weak hydrogen bonds. From crystal engineering to virtual screening.

G. R. Desiraju

Chem.Comm., 2995?3001 (2005).

268. Structural basis for bending of organic crystals.

C. M. Reddy, R. C. Gundakaram, S. Basavoju, M. T. Kirchner, K. A. Padmanabhan and G.

R. Desiraju

Chem.Comm., 3945?3947 (2005).

269. Crystal structure prediction of aminols: Advantages of a supramolecular synthon approach with experimental structures.

A. Dey, M. T. Kirchner, V. R. Vangala, G. R. Desiraju, R. Mondal and J. A. K. Howard J. Am. Chem. Soc., 127, 10545-10559 (2005).

270. Saccharin salts of active pharmaceutical ingredients, their crystal structures and increased water solubilities.

R. Banerjee, P. M. Bhatt, N. V. Ravindra, and G. R. Desiraju.

Cryst. Growth & Des., 5, 2299-2309 (2005).

271. Chemistry. The Middle Kingdom.

G. R. Desiraju

Curr. Sci., 88, 374-380 (2005).

272. Saccharin as a salt former. Enhanced solubilities of saccharinates of active pharmaceutical ingredients.

- P. M. Bhatt, N. V. Ravindra, R. Banerjee and G. R. Desiraju Chem. Comm., 1073-1075 (2005).
- 273. Structural studies of the system (Na⁺)(saccharinate²)(H2O)n. A model for crystallization. R. Banerjee, P. M. Bhatt, M. T. Kirchner and G. R. Desiraju Angew. Chem. Int. Ed., 44, 2515-2520 (2005). (VIP)
- Virtual Screening of 4-Anilinoquinazoline Analogs as EGFR Kinase Inhibitors: Importance of Hydrogen Bonds in the Evaluation of Poses and Scoring Functions.
 V. Aparna, G. Rambabu, S. K. Panigrahi, J. A. R. P. Sarma and G. R. Desiraju J. Chem. Inf. Model., 45, 725-738 (2005).
- 275. Sorting of polymorphs based on mechanical properties. Trimorphs of 6-chloro- 2,4-dinitroaniline.C. M. Reddy, S. Basavoju and G. R. Desiraju

C. M. Reddy, S. Basavoju and G. R. Desiraju Chem. Comm., 2439-2441 (2005).

276. Correlation between molecular dipole moment and centrosymmetry in some crystalline diphenyl ethers.

A. Dey and G. R. Desiraju Chem. Comm., 2486-2488 (2005).

- 277. A virtual screening approach for thymidine monophosphate kinase inhibitors as antitubercular agents based on docking and pharmacophore models.
 B. Gopalakrishnan, V. Aparna, J. Jeevan, M. Ravi and G. R. Desiraju
 J. Chem. Inf. Model., 45, 1101-1108 (2005).
- 278. C?H?O and other weak hydrogen bonds. From crystal engineering to virtual screening. G. R. Desiraju Chem.Comm., 2995?3001 (2005).
- Structural basis for bending of organic crystals.
 C. M. Reddy, R. C. Gundakaram, S. Basavoju, M. T. Kirchner, K. A. Padmanabhan and G. R. Desiraju
 Chem.Comm., 394573947 (2005).
- 280. Crystal structure prediction of aminols: Advantages of a supramolecular synthon approach with experimental structures.
 A. Dey, M. T. Kirchner, V. R. Vangala, G. R. Desiraju, R. Mondal and J. A. K. Howard J. Am. Chem. Soc., 127, 10545-10559 (2005).
- 281. Saccharin salts of active pharmaceutical ingredients, their crystal structures and increased water solubilities.
 R. Banerjee, P. M. Bhatt, N. V. Ravindra, and G. R. Desiraju.
 Cryst. Growth & Des., 5, 2299-2309 (2005).
- 282. Five varieties of hydrogen bonds in 1-formyl-3-thiosemicarbazide: An electron density study. P. Munshi, T. S. Thakur, T. N. Guru Row and G. R. Desiraju Acta Crystallogr. Sect B, 62, 118-127 (2006).
- 283. 3D-QSAR studies on antitubercular thymidine monophosphate kinase inhibitors based on different alignment methods.
 V. Aparna, J. Jeevan, M. Ravi, G. R. Desiraju and B. Gopalakrishnan Bioorg. Med. Chem. Lett., 16, 1016-1020 (2006).

- 284. Misassigned C?H···Cu agostic interaction in a copper (II) ephedrine derivative is actually a weak, multicentred hydrogen bond.
 T. S. Thakur and G. R. Desiraju
 Chem. Comm. 552-554 (2006).
- Synthon evolution and unit cell evolution during crystallisation. A study of symmetry-independent molecules (Z'>1) in crystals of some hydroxy compounds.
 D. Das, R. Banerjee, R. Mondal, J. A. K. Howard, R. Boese and G. R. Desiraju Chem. Comm., 555-557 (2006).
- 286. Isostructurality, Polymorphism and Mechanical Properties of Some Hexahalogenated Benzenes. The Nature of Halogen???Halogen Interactions.
 C. M. Reddy, M. T. Kirchner, R. C. Gundakaram, K. A. Padmanabhan and G. R. Desiraju Chem. Eur. J., 12, 2222-2234 (2006).
- Synthon Robustness and Solid-State Architecture in Substituted gem-Alkynols.
 R. Banerjee, R. Mondal, J. A. K. Howard and G. R. Desiraju
 Cryst. Growth & Des., 6, 999-1009 (2006).
- 288. Packing modes in some mono- and disubstituted phenylpropiolic acids. Repeated occurrence of the rare syn,anti-catemer.
 Dinabandhu Das and Gautam R. Desiraju
 Chem. Asian J., 1, xxx-xxx (2006). Submitted for publication.
- Ligand Coordinate Analysis of SC-558 from the Active Site to the Surface of COX-2: A Molecular Dynamics Study.
 K. V. V. M. Sai Ram, G. Rambabu, J. A. R. P. Sarma and G. R. Desiraju
 J. Chem. Inf. Model., 46, xxxx-xxxx (2006). Submitted for publication.